

# Computer algebra derives correct initial conditions for low-dimensional dynamical models

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9 June 1997

**PACS:** 02.70.Rw, 04.20.Ex, 02.30.Mv, 05.45.+b

**Keywords:** computer algebra, initial conditions, low-dimensional modelling, centre manifold, bifurcation.

## Abstract

To ease analysis and simulation we make low-dimensional models of complicated dynamical systems. Centre manifold theory provides a systematic basis for the reduction of dimensionality from some detailed dynamical prescription down to a relatively simple model. An initial condition for the detailed dynamics also has to be projected onto the low-dimensional model, but has received scant attention. Herein, based upon the reduction algorithm in [27], I develop a straightforward algorithm for the computer algebra derivation of this projection. The method is systematic and is based upon the geometric picture underlying centre manifold theory. The method is applied to examples of a pitchfork and a Hopf bifurcation. There is a close relationship between this projection of initial conditions and the correct projection of forcing onto a model. I reaffirm this connection and show how the effects of forcing, both interior and from the boundary, should be properly included in a dynamical model.

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## 1 Introduction

Ordinary differential equations or partial differential equations are used to describe dynamics in the physical world. But many modes of behaviour are of little physical interest in particular applications. The essential dynamical behaviour of the system is then determined by the evolution of a subset of the possible modes; for example, the flight of a ball is dictated solely by its velocity and spin, and hardly at all by any internal visco-elastic vibrations. Typically we say that the state of the system  $\mathbf{u}$  is some function,

$$\mathbf{u} = \mathbf{v}(\mathbf{s}), \quad (1)$$

of the few interesting modes  $\mathbf{s}$ . Then a model of the dynamics, the rigid-body dynamics of a ball for example, is governed by the low-dimensional dynamical system

$$\dot{\mathbf{s}} = \mathbf{g}(\mathbf{s}), \quad (2)$$

where the overdot denotes  $d/dt$ . Rapid damping typically characterises the modes that need to be eliminated from consideration. When many modes are heavily damped, trajectories are rapidly attracted to some low-dimensional subset of the state space, parameterized as in (1), a so-called invariant manifold [33, §1.1C]. This geometric picture of exponential collapse to a smooth invariant manifold is at the heart of the application of centre manifolds [2, 7, 26]

to the rational construction of low-dimensional models (2) by the elimination of physically uninteresting fast modes of behaviour.

The same concepts also lie behind other recent innovations in forming low-dimensional models of dynamics: inertial manifolds by Temam [30] and others; the use of centre-unstable manifolds [1, 4, 5], more general invariant manifolds [23, 24, 32] and the so-called nonlinear Galerkin method [19, 29, 11, 18, 12].

In the earlier paper [27] I reported an iterative method, based directly upon the residuals of the governing differential equations, for the construction of such low-dimensional, dynamical models. The evaluation of the residuals is a routine algebraic task which is easily programmed into computer algebra; programmed without having to become involved in all the messy details of asymptotic expansions. Two examples were discussed in [27]: a model displaying the pitchfork bifurcation of a modified Burger's equation; and the long-wave lubrication dynamics of a thin film of fluid.

However, it is not sufficient to just model the dynamics. To form a complete problem, an initial condition, say  $\mathbf{s}(0) = \mathbf{s}_0$ , has to be specified for the model (2). For very low-dimensional models with simple attractors there is perhaps little motivation, which may explain the lack of attention given to this issue. However, for models of higher dimension, initial conditions have long-lasting effects and need to be modelled correctly. This is seen in examples such as: the approach to limit cycles [34, 15]; the quasi-geostrophic approximation [17, e.g.]; long-wave models of fluid films [28, e.g.] and of dispersion in channels [20, e.g.]; and the concept of "initial slip" in some disciplines [14, 16, 13].

In [22, §2] I introduced a simple dynamical system to illustrate the correct treatment of initial conditions when forming a low-dimensional model. I now summarise that example. Consider the 2-D dynamical system

$$\dot{x} = -xy, \quad (3)$$

$$\dot{y} = -y + x^2 - 2y^2. \quad (4)$$

Linearly,  $y$  decays exponentially quickly to leave  $x$  as the dominant mode appearing in the long-term evolution. Nonlinear theory, see Carr [2] for example, asserts that the long-term evolution actually takes place on the parabolic centre manifold,  $\mathcal{M}_c$ , described parametrically as

$$x = s, \quad y = s^2. \quad (5)$$

Exponentially quickly solutions of (3–4) approach solutions on  $\mathcal{M}_c$  whose evolution is described by the *low-dimensional model*

$$\dot{s} = -s^3. \quad (6)$$

The question is: given some initial state for the detailed dynamical system (3–4), say  $(x_0, y_0)$  not on  $\mathcal{M}_c$ , what initial value of  $s$ , say  $s_0$ , is appropriate to use with the model (6) in order to guarantee fidelity between predictions of the model and the original? In [22, §2.1] I showed that this is achieved by setting

$$s_0 = x_0 - x_0(y_0 - x_0^2) + \mathcal{O}(\varepsilon^2), \quad (7)$$

where  $\varepsilon$  measures the distance from the given initial condition to the centre manifold. Alternatively, in a form we use in later generality, this projection from the given  $(x_0, y_0)$  to the correct  $(s_0, s_0^2)$  on  $\mathcal{M}_c$  is orthogonal to the vector  $\mathbf{z}(s) \approx (1, -s)$ . Only then does the predictions of the model accurately describe the long-term evolution of the original.

How in general do we find initial conditions to use with a model to make correct long-term forecasts? The Relevance Theorem of centre manifold theory [2, 27] assures us that there is indeed a particular solution of the low-dimensional model on  $\mathcal{M}_c$  which is approached exponentially by every trajectory of the full dynamical system. As developed in [22], the geometric picture of evolution near the centre manifold suggests a method of analysis. The algebra is based upon how trajectories near to the centre manifold evolve, identifying which ones approach each other exponentially quickly and thus have the same long-term evolution. For example, in the long-term dispersion down a channel [20, 32] we can discern the difference between dumping contaminant into the slow moving flow near the bank and into the fast core flow. Normal form transformations [10] also support this projection of initial conditions onto the centre manifold. In this paper I simplify the main results of [22, pp65–6], §§2.1, and in §§3.1 show how to solve the new equations using an iterative scheme based on that developed in [27] to derive the dynamical model.

However, the centre manifold based analysis reported to date has always dealt with the issue of initial conditions for models based upon *slow* modes with near zero growth rate. In general, a centre manifold model will involve the oscillating dynamics of a Hopf bifurcation or of the loss of stability to travelling waves. In §4 we also consider what extensions need to be made to the analysis and the iterative algorithm to provide correct initial conditions to models of such oscillations.

Lastly, one attribute of basic centre manifold theory is that it applies to autonomous dynamical systems. But the modelling of dynamics with time-dependent forcing is of considerable interest. In the presence of forcing a system is pushed away from the centre manifold as quantified by Cox & I [10]. Thus there is a close connection between the geometric projection of initial conditions and the appropriate projection of forcing onto the model [22,

§7]. There is also many interesting issues in the modelling of noisy dynamical systems, as expressed by stochastic differential equations [3]. In §§2.2 I reaffirm the connection and show that a new normalisation of the initial condition projection onto the centre manifold makes the projection of forcing significantly simpler. These are applied in §§3.3 to the modified Burger's dynamics to show how both interior and boundary forcing are treated. These methods should apply to interesting questions such as: what influence may turbulence have on dispersion? and how does substrate roughness affect the flow of thin films?

## 2 Geometric basis of initial condition projection

The aim of this section is to introduce some of the concepts and details of modelling initial conditions of dynamical systems. The presentation improves on earlier work reported elsewhere, predominantly in [22, 8, 3], and is adapted to a simple computational approach.

Consider a general autonomous dynamical system written in a form relative to some fixed point (taken to be the origin without loss of generality):

$$\dot{\mathbf{u}} = \mathcal{L}\mathbf{u} + \mathbf{f}(\mathbf{u}, \epsilon), \quad (8)$$

where  $\mathbf{u}(t)$  is the state vector, which may be finite or infinite dimensional,  $\mathcal{L}$  is the linear operator, and  $\mathbf{f}$  denotes all the nonlinear terms in the dynamical prescription with possible small parameters  $\epsilon$ . We suppose that  $\mathcal{L}$  has  $m$  eigenvalues with zero real-part and the remaining eigenvalues have strictly negative real-part. The linear dynamics of  $\dot{\mathbf{u}} = \mathcal{L}\mathbf{u}$  then collapse exponentially quickly onto the centre subspace  $\mathcal{E}_c$  spanned by the eigenvectors and possibly generalised eigenvectors of  $\mathcal{L}$ , namely  $\mathbf{e}_j^0$ . Nonlinear theory [2] correspondingly asserts that the exists an  $m$ -dimensional, exponentially attractive centre manifold  $\mathcal{M}_c$  which has  $\mathcal{E}_c$  as its tangent at the origin. The centre manifold is parameterized by any convenient set of  $m$  parameters, say  $\mathbf{s}$ . Thus the low-dimensional model of (8) is that

$$\mathbf{u} = \mathbf{v}(\mathbf{s}, \epsilon), \quad \text{such that} \quad \dot{\mathbf{s}} = \mathcal{G}\mathbf{s} + \mathbf{g}(\mathbf{s}, \epsilon), \quad (9)$$

where  $\mathbf{v}$  describes the shape of  $\mathcal{M}_c$ ,  $\mathcal{G}$  is a linear operator with eigenvalues all of real-part zero, and  $\mathbf{g}$  is strictly nonlinear. Theory also asserts this model is valid exponentially quickly.

In the earlier paper [27] I derived a robust and straightforward iterative algorithm to construct approximations to the model functions  $\mathbf{v}$  and  $\mathbf{g}$ . I

take this work as read. We now move on to develop the correct projection of initial conditions for (8), and then how to project a forcing superimposed on the autonomous dynamical system.

For simplicity I first assume that the critical eigenvalues of  $\mathcal{L}$  are all zero. The case of non-zero, pure imaginary eigenvalues has extra complicating details and is addressed in §4 where we investigate the specific example of a Hopf bifurcation.

## 2.1 Evolution near the centre manifold

As in [22, §5.1], consider the evolution of a point on the centre manifold,  $\mathcal{M}_c$ , and the evolution of any neighbouring point. Let  $\mathbf{n}$  denote the small vector joining these points, then, under the flow of the dynamics of (8),  $\mathbf{n}$  satisfies the linear equation

$$\frac{d\mathbf{n}}{dt} = \mathcal{J}\mathbf{n}, \quad \text{where } \mathcal{J} = \mathcal{L} + \mathcal{N}, \quad (10)$$

is the Jacobian of (8) evaluated on  $\mathcal{M}_c$  and where  $\mathcal{N} = \partial\mathbf{f}/\partial\mathbf{u}$  is the Jacobian of the nonlinear and parameter dependent terms. Note that  $\mathcal{N}$  and hence  $\mathcal{J}$  are functions of position  $\mathbf{s}$  on the centre manifold. It is useful to imagine any given  $\mathbf{n}$  to be a function of position on  $\mathcal{M}_c$  rather than time; in this case we deduce by the chain rule that

$$\frac{d\cdot}{dt} = \frac{\partial\cdot}{\partial\mathbf{s}} (\mathcal{G}\mathbf{s} + \mathbf{g}) = (\mathcal{G}_{jk}s_k + g_j) \frac{\partial}{\partial s_j},$$

using the summation convention hereafter. The projection of initial conditions onto  $\mathcal{M}_c$  is done along what have been termed “isochronic manifolds”, denoted herein by  $\mathcal{I}$ . Such a projection of initial conditions is also supported by normal form transformations as discussed Cox & Roberts [10]. The most well known isochronic manifold is simply the stable manifold of the origin,  $\mathcal{M}_s$ : since the origin is an equilibrium in the model, that trajectories starting on  $\mathcal{M}_s$  exponentially quickly approach the origin is precisely the requirement for the isochronic manifold of the origin’s fixed dynamics.

Under the evolution in the neighbourhood of  $\mathcal{M}_c$  the displacement vector  $\mathbf{n}$  will do either of two things: the tip of  $\mathbf{n}$  off the manifold will approach  $\mathcal{M}_c$  exponentially quickly but in general it will have slipped from the base point on  $\mathcal{M}_c$  and thus  $\mathbf{n}$  will exponentially quickly become tangent to  $\mathcal{M}_c$ ; alternatively, if  $\mathbf{n}$  is aligned just right then the tip will approach the base while remaining transverse to  $\mathcal{M}_c$ . It is this latter case that is of interest as an initial condition of the full dynamics at the tip of  $\mathbf{n}$  will result in a

long-term evolution that is indistinguishable from that of the evolution of the base point. Thus the base point forms the appropriate initial condition for the low-dimensional dynamics on  $\mathcal{M}_c$ . The set of all such tip points that exponentially approach  $\mathcal{M}_c$ , while  $\mathbf{n}$  remains transverse, forms the isochronic manifold  $\mathcal{I}$  for any specified initial condition on  $\mathcal{M}_c$ .

To describe the projection of given initial conditions  $\mathbf{u}_0$  of the full dynamics onto  $\mathcal{M}_c$ , we use the normal vectors to the isochronic manifolds. More specifically we use the normal vectors of  $\mathcal{I}$  at  $\mathcal{M}_c$ . Let  $\mathbf{n}_\alpha = \mathbf{u}_0 - \mathbf{v}(\mathbf{s}_0, \epsilon)$  be a family of small vectors which span the tangent space of  $\mathcal{I}$ . Then in terms of an inner product  $\langle \cdot, \cdot \rangle$ , we seek  $m$  linearly independent vectors, say  $\mathbf{r}_i$  as a function of position  $\mathbf{s}$ , such that

$$\langle \mathbf{r}_i, \mathbf{n}_\alpha \rangle = 0. \quad (11)$$

It is much easier to find the  $m$  vectors  $\mathbf{r}_i$  than the possible infinity of vectors  $\mathbf{n}_\alpha$ . Taking  $d/dt$  of (11) and using (10) we deduce

$$\mathcal{D}\mathbf{r}_i = \mathbf{0} \quad \text{where} \quad \mathcal{D} = \frac{d}{dt} + \mathcal{J}^\dagger, \quad (12)$$

and  $\mathcal{J}^\dagger$  denotes the adjoint in the specified inner product. This equation describes how the normal vectors  $\mathbf{r}_i$  vary over  $\mathcal{M}_c$ . Call  $\mathcal{D}$  the *dual*.

We need to solve (12). But in general  $\mathbf{r}_i$  will inconveniently vary quickly in magnitude and possibly direction over  $\mathcal{M}_c$ . Whereas all we are actually interested in is the space spanned by  $\mathbf{r}_i$ , namely the tangent space to  $\mathcal{I}$  at  $\mathcal{M}_c$ . Instead we seek an equivalent basis for  $\mathcal{I}$ , one which varies relatively slowly over  $\mathcal{M}_c$ , by the invertible transformation  $\mathbf{r}_i = Q_{ij}\mathbf{z}_j$  for some basis vectors  $\mathbf{z}_j$  also a function of position on  $\mathcal{M}_c$ . It is from here that we depart significantly from the analysis reported in my earlier work [22, §5]. For a reason that becomes apparent in the next subsection, we seek the particular basis such that

$$\langle \mathbf{z}_i, \mathbf{e}_j \rangle = \delta_{ij} \quad \text{where} \quad \mathbf{e}_j(\mathbf{s}, \epsilon) = \frac{\partial \mathbf{v}}{\partial s_j} \quad (13)$$

are local tangent vectors to  $\mathcal{M}_c$  based upon the parameterization of  $\mathcal{M}_c$ ; typically  $\mathbf{e}_j \rightarrow \mathbf{e}_j^0$  as  $(\mathbf{s}, \epsilon) \rightarrow \mathbf{0}$ . Substituting  $\mathbf{r}_i = Q_{ij}\mathbf{z}_j$  into (12) then leads to

$$\begin{aligned} & \frac{dQ_{ij}}{dt} \mathbf{z}_j + Q_{ij} \mathcal{D} \mathbf{z}_j = \mathbf{0} \\ \Rightarrow & \frac{dQ_{ik}}{dt} + Q_{ij} \langle \mathcal{D} \mathbf{z}_j, \mathbf{e}_k \rangle = 0 \quad \text{upon taking } \langle \cdot, \mathbf{e}_k \rangle \\ \Rightarrow & -Q_{ij} \langle \mathcal{D} \mathbf{z}_j, \mathbf{e}_k \rangle \mathbf{z}_k + Q_{ij} \mathcal{D} \mathbf{z}_j = \mathbf{0} \quad \text{putting } dQ_{ij}/dt \text{ in the first.} \end{aligned}$$

But  $Q_{ij}$  is an invertible matrix and thus we must solve

$$\mathcal{D}\mathbf{z}_j - \langle \mathcal{D}\mathbf{z}_j, \mathbf{e}_k \rangle \mathbf{z}_k = \mathbf{0}, \quad (14)$$

in conjunction with the orthonormality condition (13) in order to find the basis vectors  $\mathbf{z}_j$  for the isochronic manifolds  $\mathcal{I}$ .

Equation (14) has a reasonable interpretation. The second term just projects the residual of the dual (12) onto  $\mathcal{I}$ , and hence (14) requires all other components of the residual to be zero. Thus (14) requires that the basis indeed twists with  $\mathcal{I}$ , but places no restraint on how the basis spans  $\mathcal{I}$ ; the orthonormality condition (13) closes the problem to give a unique solution.

Once the basis vectors  $\mathbf{z}_j$  are found, we then solve

$$\langle \mathbf{z}_j(\mathbf{s}_0, \epsilon), \mathbf{u}_0 - \mathbf{v}(\mathbf{s}_0, \epsilon) \rangle = 0 \quad \text{for all } j \quad (15)$$

to determine the projection of a given initial state  $\mathbf{u}_0$  onto an initial state  $\mathbf{s}_0$  for the model (9). This projection is linear in distance away from the centre manifold  $\mathcal{M}_c$ . There will be errors quadratic in the distance. However, in many applications the stable manifold  $\mathcal{M}_s$  is precisely the linear stable subspace  $\mathcal{E}_s$ ; hence at least near the origin we may expect that a linear projection onto  $\mathcal{M}_c$  will be quite good.

## 2.2 Model forcing by the same projection

In this subsection we consider the dynamical system (8) with a small, of  $\mathcal{O}(\epsilon)$ , forcing superimposed. Namely we analyse briefly

$$\dot{\mathbf{u}} = \mathcal{L}\mathbf{u} + \mathbf{f}(\mathbf{u}, \epsilon) + \epsilon\mathbf{p}(\mathbf{u}, t, \epsilon), \quad (16)$$

for small forcing  $\epsilon\mathbf{p}$ . The forcing could be deterministic, as investigated by Cox & I [22, 8], or stochastic as examined by Chao & I [3]. Our aim is to transform the forcing of the detailed system (16) into a corresponding forcing of the model (9). That is, we seek the forced centre manifold and the evolution thereon in the form

$$\begin{aligned} \mathbf{u} &= \mathbf{v}(\mathbf{s}, \epsilon) + \epsilon\mathbf{w}(\mathbf{s}, t, \epsilon) + \mathcal{O}(\epsilon^2), \\ \text{s.t. } \dot{\mathbf{s}} &= \mathcal{G}\mathbf{s} + \mathbf{g}(\mathbf{s}, \epsilon) + \epsilon\mathbf{q}(\mathbf{s}, t, \epsilon) + \mathcal{O}(\epsilon^2), \end{aligned} \quad (17)$$

where  $\mathbf{w}$  describes the displacement of  $\mathcal{M}_c$  and  $\mathbf{q}$  is our main interest as it describes the correct forcing to be used in the model.

That the projection of a forcing onto a model is nontrivial was shown in [22, §7.1]. There a steady forcing of  $-\varepsilon$  in the  $y$  equation (4) of the simple system (3–4) results in the model

$$\dot{s} = -s^3 + \varepsilon s,$$

which exhibits the destabilization of the origin in favour of either of two fixed points at  $s = \pm\sqrt{\varepsilon}$ . This result is remarkable in that the response is comparatively large, of  $\mathcal{O}(\sqrt{\varepsilon})$ , when the original forcing is normal to  $\mathcal{E}_c$  and so usually would be neglected by heuristic arguments.

In [22, §7] I argued that the projection of initial conditions could be used to deduce how to model forcing. This close connection between the two processes was supported by further work by Cox & I [8]. Here I briefly reaffirm the connection and show why the orthonormality condition (13) is desirable.

To find an equation for  $\mathbf{q}$ , simply substitute (17) into the original system (16) and group all terms linear in  $\varepsilon$  to deduce

$$\frac{d\mathbf{w}}{dt} + \mathcal{E}\mathbf{q} = \mathcal{J}\mathbf{w} + \mathbf{p}, \quad (18)$$

where  $\mathcal{E} = [\mathbf{e}_j]$  is the matrix of tangent vectors, and here

$$\frac{d\cdot}{dt} = \frac{\partial\cdot}{\partial t} + \frac{\partial\cdot}{\partial s} (\mathcal{G}\mathbf{s} + \mathbf{g}),$$

due to the direct dependency upon time introduced by the forcing  $\mathbf{p}(\mathbf{u}, t)$ . Taking  $\langle \mathbf{z}_i, \cdot \rangle$  of this equation and using the adjoint properties we must have

$$\frac{d}{dt} \langle \mathbf{z}_i, \mathbf{w} \rangle - \langle \frac{d\mathbf{z}_i}{dt}, \mathbf{w} \rangle + \langle \mathbf{z}_i, \mathbf{e}_j \rangle q_j = \langle \mathcal{J}^\dagger \mathbf{z}_i, \mathbf{w} \rangle + \langle \mathbf{z}_i, \mathbf{p} \rangle. \quad (19)$$

Using the orthonormality (13),  $\langle \mathbf{z}_i, \mathbf{e}_j \rangle q_j = q_i$ . Without loss of generality, choose the parameterization of positions near  $\mathcal{M}_c$  so that

$$\langle \mathbf{z}_i, \mathbf{w} \rangle = 0. \quad (20)$$

Indeed, Cox & I [8] showed that this is the *only* choice for  $\mathbf{w}$  that removes clumsy history dependent integrals from the forcing  $\mathbf{q}$  of the model. Thus (19) becomes

$$q_i = \langle \mathbf{z}_i, \mathbf{p} \rangle + \langle \frac{d\mathbf{z}_i}{dt} + \mathcal{J}^\dagger \mathbf{z}_i, \mathbf{w} \rangle.$$

The last term involves  $\mathcal{D}\mathbf{z}_i$  which, by the projected dual (14), must lie in the space spanned by the  $\mathbf{z}_k$ 's, is thus orthogonal to  $\mathbf{w}$ , and so the last term

vanishes. Hence the appropriate linear approximation to the forcing of the model is simply the projection

$$q_i = \langle \mathbf{z}_i, \mathbf{p} \rangle, \quad (21)$$

for any given forcing  $\mathbf{p}$  in terms of the vectors  $\mathbf{z}_i$  determined for the projection of initial conditions.

### 3 Initial conditions—a pitchfork bifurcation

In [27] I described a simple and robust iterative scheme for the computer algebra derivation of the dynamical model (9) from the detailed system (8). In this section I describe how to extend the iterative scheme to derive the projection of initial conditions. This scheme is also eminently suitable for computer algebra and I illustrate its application by using the iteration to determine initial conditions for the relatively simple pitchfork bifurcation dynamics in a specific infinite dimensional dynamical system. Here we consider the simpler case of centre manifold models formed when the critical eigenvalues are precisely zero, rather than the more complicated case of non-zero imaginary part considered in the next section.

A summary of the iteration for the centre manifold model is as follows. Suppose we know an approximation to  $\mathcal{M}_c$  and the evolution thereon, namely

$$\mathbf{u} \approx \tilde{\mathbf{v}}(\mathbf{s}, \epsilon) \quad \text{s.t.} \quad \dot{\mathbf{s}} \approx \mathcal{G}\mathbf{s} + \tilde{\mathbf{g}}(\mathbf{s}, \epsilon).$$

For example, usually we start the iteration with the linear approximation:  $\tilde{\mathbf{v}} = \mathcal{E}^0 \mathbf{s}$  and  $\tilde{\mathbf{g}} = \mathbf{0}$ . Then we seek an improved description, that

$$\mathbf{u} \approx \tilde{\mathbf{v}} + \mathbf{v}' \quad \text{s.t.} \quad \dot{\mathbf{s}} \approx \mathcal{G}\mathbf{s} + \tilde{\mathbf{g}} + \mathbf{g}',$$

where primes indicate small correction terms to be determined. Substituting into the governing differential equation (8), neglecting products of small quantities, and approximating coefficients of primed quantities by their zeroth order approximation, we deduce that the corrections satisfy

$$\frac{\partial \tilde{\mathbf{v}}}{\partial \mathbf{s}}(\mathcal{G}\mathbf{s} + \tilde{\mathbf{g}}) + \mathcal{E}^0 \mathbf{g}' + \frac{\partial \mathbf{v}'}{\partial \mathbf{s}} \mathcal{G}\mathbf{s} = \mathcal{L}\tilde{\mathbf{v}} + \mathcal{L}\mathbf{v}' + \mathbf{f}(\tilde{\mathbf{v}}, \epsilon).$$

It is not obvious, but provided the definition of amplitudes are arranged so that  $\mathcal{G}$  is in Jordan form, we may significantly simplify the algorithm by also neglecting the term  $\frac{\partial \mathbf{v}'}{\partial \mathbf{s}} \mathcal{G}\mathbf{s}$ . (It is often physically appealing to use the Jordan form because, for example, the two amplitudes involved often represent the

“position” and “momentum” of a specific mode.) Thus, rearranging and recognising that

$$\frac{\partial \tilde{\mathbf{v}}}{\partial \mathbf{s}}(\mathcal{G}\mathbf{s} + \tilde{\mathbf{g}}) = \frac{d\tilde{\mathbf{v}}}{dt}$$

by the chain rule for the current approximation, we solve

$$\mathcal{L}\mathbf{v}' - \mathcal{E}^0\mathbf{g}' = \frac{d\tilde{\mathbf{v}}}{dt} - \mathcal{L}\tilde{\mathbf{v}} - \mathbf{f}(\tilde{\mathbf{v}}, \epsilon). \quad (22)$$

Recognise that the right-hand side is simply the residual of the governing equation (8) evaluated at the current approximation. Thus at any iteration we just deal with physically meaningful expressions; all the complicated rearrangements of asymptotic expansions as needed by earlier methods are absent. All the messy algebra in the repeated evaluation of the residuals may be left to the computer to perform—such mindless repetition is ideal for a computer—whereas all a human need concern themselves with is setting up the typical solution of

$$\mathcal{L}\mathbf{v}' - \mathcal{E}^0\mathbf{g}' = \text{residual},$$

and not at all with the detailed algebraic machinations of asymptotic expansions.

Consider the following variation to Burger’s equation featuring growth,  $(1 + \epsilon)u$ , nonlinearity,  $uu_x$ , and dissipation,  $u_{xx}$ :

$$\frac{\partial u}{\partial t} = (1 + \epsilon)u + u\frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2}, \quad u(0, t) = u(\pi, t) = 0, \quad (23)$$

for some function  $u(x, t)$ . View this as an infinite dimensional dynamical system, the state space being the set of all functions  $u(x)$  on  $[0, \pi]$ . The above iteration scheme may be employed to find the centre manifold dynamics near the bifurcation that takes place as  $\epsilon$  crosses zero. This application is described in detail in [27]: lines 1–29 of the REDUCE<sup>1</sup> computer algebra program listed in §§3.2 tell us that the centre manifold is

$$u = a \sin(x) + \frac{1 - \epsilon/3}{6}a^2 \sin(2x) + \frac{1 - 7\epsilon/12}{32}a^3 \sin(3x) + \mathcal{O}(\epsilon^2, a^4), \quad (24)$$

when parameterized by  $a$ , the amplitude of the  $\sin(x)$  component of  $u$ . Upon this centre manifold the low-dimensional model is that

$$\dot{a} = \epsilon a - \frac{1 - \epsilon/3}{12}a^3 + \mathcal{O}(\epsilon^2, a^4). \quad (25)$$

This model, for example, predicts the pitchfork bifurcation as  $\epsilon$  crosses zero.

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<sup>1</sup>At the time of writing, information about REDUCE was available from Anthony C. Hearn, RAND, Santa Monica, CA 90407-2138, USA. E-mail: [reduce@rand.org](mailto:reduce@rand.org)

### 3.1 Iterative algorithm for the projection

Having outlined the iteration scheme to find the centre manifold model, we now turn to implementing a similar but novel iteration scheme to determine the vectors  $\mathbf{z}_j$  that govern the projection of initial conditions. The scheme is illustrated by applying it to the pitchfork bifurcation in (23).

We need to solve (14) subject to the orthonormality condition (13). The method of solution is to iteratively improve an approximation based upon the residuals of the equations. We start the iteration with the linear approximation that  $\mathbf{z}_j$  are eigenvectors or generalised eigenvectors,  $\mathbf{z}_j^0$ , of  $\mathcal{L}^\dagger$ , the adjoint linear operator. Suppose that at some later stage we know an approximation  $\mathbf{z}_j \approx \tilde{\mathbf{z}}_j$ , we then seek an improved approximation

$$\mathbf{z}_j \approx \tilde{\mathbf{z}}_j + \mathbf{z}'_j. \quad (26)$$

Firstly, substituting into the orthonormality condition (13) gives

$$\langle \mathbf{z}'_i, \mathbf{e}_j \rangle = \delta_{ij} - \langle \tilde{\mathbf{z}}_i, \mathbf{e}_j \rangle.$$

Approximating the coefficient of the primed correction quantity then shows that we impose on  $\mathbf{z}'_i$  the requirement that

$$\langle \mathbf{z}'_i, \mathbf{e}_j^0 \rangle = \delta_{ij} - \langle \tilde{\mathbf{z}}_i, \mathbf{e}_j \rangle. \quad (27)$$

Secondly, substituting (26) into the projected dual equation (14) and dropping products of correction terms gives

$$-\mathcal{D}\mathbf{z}'_j + \langle \mathcal{D}\tilde{\mathbf{z}}_j, \mathbf{e}_k \rangle \mathbf{z}'_k + \langle \mathcal{D}\mathbf{z}'_j, \mathbf{e}_k \rangle \tilde{\mathbf{z}}_k = \mathcal{D}\tilde{\mathbf{z}}_j - \langle \mathcal{D}\tilde{\mathbf{z}}_j, \mathbf{e}_k \rangle \tilde{\mathbf{z}}_k. \quad (28)$$

Approximating all coefficients of primed quantities, all appearing on the left-hand side, by their zeroth-order approximation, we seek a correction such that

$$-\mathcal{L}^\dagger \mathbf{z}'_j + \langle \mathcal{L}^\dagger \mathbf{z}_j^0, \mathbf{e}_k^0 \rangle \mathbf{z}'_k + \langle \mathcal{L}^\dagger \mathbf{z}'_j, \mathbf{e}_k^0 \rangle \mathbf{z}_k^0 = \mathcal{D}\tilde{\mathbf{z}}_j - \langle \mathcal{D}\tilde{\mathbf{z}}_j, \mathbf{e}_k \rangle \tilde{\mathbf{z}}_k.$$

The two inner products on the left-hand side vanish as they both may be transformed to a form  $\langle \cdot, \mathcal{L}\mathbf{e}_k^0 \rangle$  which is zero as  $\mathbf{e}_k^0$  is a critical eigenvector of  $\mathcal{L}$ . Thus we solve the linear equation

$$-\mathcal{L}^\dagger \mathbf{z}'_j = \mathcal{D}\tilde{\mathbf{z}}_j - \langle \mathcal{D}\tilde{\mathbf{z}}_j, \mathbf{e}_k \rangle \tilde{\mathbf{z}}_k, \quad (29)$$

for the corrections  $\mathbf{z}'_j$ . Thus the corrections are simply driven by the residual of the projected dual (14) evaluated at the current approximation as appears on the right-hand side of (29). One uncomfortable feature of (29) is that sometimes during the course of the iteration there is a component of  $\mathbf{z}_k^0$  in the right-hand side—it should be ignored and ultimately it will vanish as the iteration proceeds.

### 3.2 The example pitchfork bifurcation

A principal reason for adopting this approach is because the iteration is simply implemented in computer algebra. I discuss the implementation of the iterative algorithm when applied to determining initial conditions for the model (25) of the modified Burger's equation (23).

Based upon the above derivation, the general outline of the algorithm is:

1. find the centre manifold and the evolution thereon;
2. initialisation and linear approximation;
3. repeat until residuals are small enough;
  - (a) compute normality and adjoint residuals,
  - (b) compute projected adjoint residual,
  - (c) solve for the correction and update approximation.

In practise, the iteration for the initial condition projection could be intertwined with the iteration for the centre manifold model. However, here we keep them separate for clarity.

Implemented in REDUCE for Burger's equation (23) the algorithm may look like the second part of the following.

```

1 COMMENT First find pitchfork bifurcation in u_t=(1+eps)u+uu_x+u_xx,
2 where a(t) measures amplitude of sin(x) component in u(x,t)
3 ;
4 on div; off allfac; on revpri; factor sin; % improve print appearance
5 % trigonometry rules OK
6 let { sin(~x)*cos(~y) => (sin(x+y)+sin(x-y))/2
7      , sin(~x)*sin(~y) => (-cos(x+y)+cos(x-y))/2
8      , sin(~x)^2 => (-cos(2*x)+1)/2};
9 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
10 % Define the inverse operator of u+u_xx
11 operator linv; linear linv;
12 let linv(sin(~k*x),x) => sin(k*x)/(1-k^2);
13 % Using inner product: <u,v>=(2/pi)\int_0^pi u.v dx
14 operator mmean; linear mmean;
15 let { mmean(1,x)=>2, mmean(cos(x),x)=>0, mmean(cos(~k*x),x)=>0 };
16 %
17 depend a,t;          % asserts that a depends upon time t
18 let df(a,t) => g;    % so da/dt is replaced by current g(a,eps)
19 %
20 u:=a*sin(x); g:=0;   % initial approximation
21 %
22 % iterate until PDE is satisfied (to requisite order)
23 let {eps^2=0, a^4=0}; % discard high-order terms in a & eps

```

```

24 repeat begin
25   write eqn:=df(u,t)-(1+eps)*u-u*df(u,x)-df(u,x,x);
26   gd:=-mmean(sin(x)*eqn,x);
27   write u:=u+linv(eqn+sin(x)*gd,x);
28   write g:=g+gd;
29 end until eqn=0;
30 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
31 % Second find projection of initial conditions onto centre manifold
32 % Get tangent vector to centre manifold for normalisation
33 write es:=df(u,a);
34 % Define the adjusted inverse of adjoint operator of u+u_xx
35 operator lainv; linear lainv;
36 let {lainv(sin(~k*x),x) => sin(k*x)/(1-k^2), lainv(sin(x),x)=>0};
37 % linear approximation to projection kernel, then iterate
38 z:=sin(x);
39 repeat begin
40   write norm:=mmean(z*es,x)-1;
41   dz:= df(z,t)+(1+eps)*z-u*df(z,x)+df(z,x,2);
42   write eqn:=dz-mmean(dz*es,x)*z;
43   write z:=z-lainv(eqn,x)-norm*sin(x);
44 end until (eqn=0)and(norm=0);
45 end;

```

Observe the how lines 32–44 of this program implements the algorithm for the initial condition projection.

1.  $\ell_{4-29}$  find the centre manifold and the evolution thereon using the iterative algorithm of [27] as outlined at the start of §3;

2.  $\ell_{33-38}$  Initialisation.

- $\ell_{33}$ , the local tangent vector to  $\mathcal{M}_c$ , namely

$$e(x) = \sin x + \frac{1}{3}a \sin(2x) + \frac{3}{32}a^2 + \mathcal{O}\left(a^3 + \epsilon^{3/2}\right),$$

- $\ell_{35-36}$  defines `lainv`, the inverse of the adjoint operator  $\mathcal{L}^\dagger$ . Here, under the obvious inner product

$$\langle u, v \rangle = \frac{2}{\pi} \int_0^\pi uv \, dx,$$

$\mathcal{L}$  is self adjoint so `lainv` is identical to `linv`, except that we need to neglect any component in  $z^0(x) = e^0(x) = \sin x$  as commented upon earlier.

- $\ell_{38}$  gives the initial linear approximation to the projection

$$z \approx z^0 = \sin x.$$

3.  $\ell39\text{--}44$  perform the iteration until the residuals are negligible according to the `let` statement of  $\ell23$ ;

- $\ell40\text{--}41$  compute normality (13) and dual (12) residuals for the current approximation direct from their equations,
- $\ell42$  computes the projected dual residual (14),
- $\ell43$  solves for the correction and updates the approximation to the projection vector  $z(x)$ .

Running this program shows that

$$\begin{aligned} z = & \left(1 + \frac{a^2}{18}\right) \sin x - \frac{1 + \epsilon/3}{6} a \sin(2x) + \frac{1 + 5\epsilon/4}{96} a^2 \sin(3x) \\ & + \mathcal{O}(a^3, \epsilon^2). \end{aligned} \quad (30)$$

The task of finding the correct initial condition for the model (25) is then the following. Given an initial condition for the Burger's equation (23), namely that  $u = u_0(x)$  at  $t = 0$ , we project onto the centre manifold by solving for the amplitude  $a_0$  in the nonlinear equation

$$\langle z(a_0, x), u_0(x) - v(a_0, x) \rangle = 0. \quad (31)$$

An iterative approach will usually suffice to solve this. Starting with the approximation  $\tilde{a}_0 = \langle z^0, u_0 \rangle$ , successive corrections may be computed as

$$a'_0 = \langle z(\tilde{a}_0, x), u_0(x) - v(\tilde{a}_0, x) \rangle.$$

For example, if  $u_0 = \alpha \sin x$  for some particular  $\alpha$ , then

$$a_0 = \alpha + \frac{1}{36} \alpha^3 + \mathcal{O}(\alpha^4, \epsilon^2), \quad (32)$$

and *not* simply  $a_0 = \alpha$  as would be implied by a direct application of the definition of amplitude  $a$ .

Of course in this particular application the issue of the precisely correct initial condition is of little interest because the ultimate fate of the dynamics is absorption by a stable fixed point and an incorrect initial condition just causes a small error in the timing of the approach. However, in more complicated dynamical models with non-trivial long-term dynamics, for example in chaotic models or in the shear dispersion of contaminant in a pipe or channel, errors in the initial condition can cause significant long-term errors in the predictions of a model. But before moving on to the analysis of such a problem, we investigate in the next subsection the projection of forcing in this modified Burger's equation (23).

### 3.3 Forcing in the interior and on boundaries

The forced equation we consider briefly in this subsection is (23) with some unspecified small forcing  $\varepsilon p(u, x, t)$ , namely

$$\frac{\partial u}{\partial t} = (1 + \epsilon)u + u\frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2} + \varepsilon p(u, x, t). \quad (33)$$

Then by the arguments of §2.2 the forcing of the model (25) turns it into

$$\dot{a} = \epsilon a - \frac{1 - \epsilon/3}{12}a^3 + \langle z, \varepsilon p(v, x, t) \rangle + \mathcal{O}(\epsilon^2, a^4, \varepsilon^2). \quad (34)$$

For example, a spatially uniform, additive forcing  $\varepsilon p(t)$  induces a multiplicative forcing as in

$$\dot{a} = \epsilon a - \frac{1 - \epsilon/3}{12}a^3 + \left( \frac{4}{\pi} + \frac{17 + 5\epsilon/4}{72\pi}a^2 \right) \varepsilon p + \mathcal{O}(\epsilon^2, a^4, \varepsilon^2).$$

Also, as in the example near the start of §2.2, here a forcing proportional to  $\sin(2x)$  may destabilize the origin.

The above results on forcing in the interior of the domain are straightforward given the analysis of §2.2. A little more subtle is the effects of forcing in the boundary conditions. For example, (33) may have forced boundary conditions such as

$$u(0, t) = \varepsilon p_0(t), \quad u(\pi, t) = \varepsilon p_\pi(t). \quad (35)$$

For the moment, assume there is no forcing in the interior—these are the only forcing terms.

One heuristic approach is to turn these boundary conditions into interior Dirac delta function forcing of the same problem but with homogeneous boundary conditions. In essence, this approach forces an extremely thin boundary layer at  $x = 0^+$  between the boundary value of  $u(0) = 0$  and an interior value of  $u(0^{++}) = \varepsilon p_0$ , and similarly near  $x = \pi$ . We try the forcing  $\varepsilon p = A\delta'(x - 0^+) + B\delta'(x - \pi^-)$  in (33) with the homogeneous boundary conditions of (23). Here  $\delta'(x)$  denotes the derivative of the Dirac delta function. Then integrating  $x$  times (33) over the extremely small interval  $[0, 0^{++}]$  leads to  $u(0^{++}) = -A$  as the effective boundary value of  $u$  at  $x = 0$ . Similar integration near  $x = \pi$  leads to  $u(\pi^{--}) = B$  as an effective boundary value. Thus to match the forced boundary conditions (35), we choose

$$\varepsilon p(x, t) = -\varepsilon p_0(t)\delta'(x - 0^+) + \varepsilon p_\pi(t)\delta'(x - \pi^-). \quad (36)$$

Then the projection of such an “interior” forcing onto the model, equation (34), leads to

$$\begin{aligned}\dot{a} = & \epsilon a - \frac{1-\epsilon/3}{12}a^3 + \frac{2}{\pi} \left(1 + \frac{25}{288}a^2\right) \varepsilon(p_\pi + p_0) \\ & + \frac{1+\epsilon/3}{3\pi}a\varepsilon(p_\pi - p_0) + \mathcal{O}(\epsilon^2, a^3, \varepsilon^2).\end{aligned}\quad (37)$$

Notice that an asymmetry in the boundary forcing,  $p_\pi \neq p_0$ , may destabilize the fixed point at the origin.

Another more systematic approach identifies where inhomogeneous boundary conditions such as (35) affect the earlier analysis. We now do this. Realise that with forcing in the boundaries the differential Jacobian term  $\mathcal{J}w$  in (18) then comes with the attached boundary conditions that  $w(0, t) = p_0$  and  $w(\pi, t) = p_\pi$ . Consequently, here the integration by parts in going from (18) to (19) introduces extra terms as

$$\langle z, \mathcal{J}w \rangle = \langle \mathcal{J}^\dagger z, w \rangle - \frac{2}{\pi} [z_x w]_0^\pi.$$

Hence the forcing of the model is not just the projection of the interior forcing,  $\langle z, p \rangle$ , but instead contains extra terms:

$$q = \langle z, p \rangle + \frac{2}{\pi} [z_x(0)p_0(t) - z_x(\pi)p_\pi(t)]. \quad (38)$$

After substituting in the expression (30) for  $z$ , this agrees precisely with (37).

## 4 Correct phase near a Hopf bifurcation

In the analysis and example of the previous sections, the dynamics on the centre manifold have been based on the critical eigenvalues being precisely 0, not the more general case where just the real part of the eigenvalues are zero but the imaginary part is non-zero. However, because an eigenvalue with a non-zero imaginary part is always associated with oscillations, such a case is important in practise as it arises in the common transition from steady to oscillatory dynamics. Because it is significantly more difficult to determine the projection of initial conditions for such oscillatory dynamics, I describe a specific implementation in this section. Note that in a Hopf bifurcation, as recognised by Winfree [34] and Guckenheimer [15], unless a good initial condition is found the phase between the model and the actual dynamics are irretrievably different.

As an example, consider the dynamics of the following dynamical system

$$\dot{\mathbf{u}} = \begin{bmatrix} -1 & -1 & 0 \\ 2 & 1 & 0 \\ 1 & 2 & -1 \end{bmatrix} \mathbf{u} + \begin{bmatrix} \epsilon u_1 - 2u_1 u_3 \\ 2u_1 u_3 \\ u_2^2 \end{bmatrix}, \quad (39)$$

where  $\epsilon$  is a control parameter. It is straightforward to discover that when  $\epsilon$  is zero, the critical value, the linear operator has eigenvalues  $\pm i$  and  $-1$ . Thus there exists a centre manifold corresponding to the two eigenvalues  $\pm i$ . The mode with eigenvalue  $-1$  is representative of the many exponentially decaying modes we find in real applications.

## 4.1 The example centre manifold model

Our interest herein lies in the provision of correct initial conditions for a low-dimensional model, not immediately in the construction of the model. Hence, in this subsection I record the principal features of the centre manifold model of (39) and do not describe its derivation.

The eigenvectors corresponding to the critical eigenvalues enables us to construct the centre eigenspace,  $\mathcal{E}_c$ , the linear approximation to the centre manifold. The eigenvectors of  $\lambda = \pm i$  are  $(2, -2 \pm 2i, -3 \pm i)$  and we use the real and imaginary parts of these eigenvectors to span  $\mathcal{E}_c$ . A linear approximation to the centre manifold is then

$$\mathcal{E}_c = \left\{ x\mathbf{e}_x^0 + y\mathbf{e}_y^0 \mid \forall x, y \right\} \quad \text{where} \quad \mathbf{e}_x^0 = \begin{bmatrix} 2 \\ -2 \\ -3 \end{bmatrix}, \quad \mathbf{e}_y^0 = \begin{bmatrix} 0 \\ 2 \\ 1 \end{bmatrix}.$$

Then in terms of  $\mathbf{s} = (x, y)$ , the linear dynamics on the centre manifold are the oscillations described by

$$\dot{\mathbf{s}} = \mathcal{G}\mathbf{s}, \quad \text{where} \quad \mathcal{G} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}. \quad (40)$$

In a general problem the centre subspace is described by  $\mathbf{u} = \mathbf{e}_j^0 s_j$ . Hence the linear evolution equation  $d\mathbf{u}/dt = \mathcal{L}\mathbf{u}$  becomes

$$\mathcal{L}\mathbf{e}_k^0 s_k = \frac{d\mathbf{u}}{dt} = \mathbf{e}_j^0 \frac{ds_j}{dt} \approx \mathbf{e}_j^0 \mathcal{G}_{jk} s_k.$$

Since this holds for all sufficiently small  $s_k$ , we deduce the generalised basis vectors for the centre subspace satisfy

$$\mathcal{L}\mathbf{e}_k^0 = \mathbf{e}_j^0 \mathcal{G}_{jk}. \quad (41)$$

Similarly look at the linear equation for the leading order projection vectors  $\mathbf{z}_j^0$ . At leading order the projected dual (14) becomes

$$\mathcal{L}^\dagger \mathbf{z}_j^0 - \langle \mathcal{L}^\dagger \mathbf{z}_j^0, \mathbf{e}_k^0 \rangle \mathbf{z}_k^0 = 0,$$

after dropping  $d\mathbf{z}_j/dt$  and  $\mathcal{N}^\dagger \mathbf{z}_j$  as being small. Then

$$\begin{aligned} \mathcal{L}^\dagger \mathbf{z}_j^0 &= \langle \mathcal{L}^\dagger \mathbf{z}_j^0, \mathbf{e}_k^0 \rangle \mathbf{z}_k^0 \\ &= \langle \mathbf{z}_j^0, \mathcal{L} \mathbf{e}_k^0 \rangle \mathbf{z}_k^0 \quad \text{by adjoint property} \\ &= \langle \mathbf{z}_j^0, \mathbf{e}_\ell^0 \mathcal{G}_{\ell k} \rangle \mathbf{z}_k^0 \quad \text{by (41)} \\ &= \delta_{j\ell} \mathcal{G}_{\ell k} \mathbf{z}_k^0 \quad \text{by orthonormality (13)} \end{aligned}$$

Thus the initial approximation for the projection vectors must satisfy

$$\mathcal{L}^\dagger \mathbf{z}_j^0 = \mathcal{G}_{jk} \mathbf{z}_k^0. \quad (42)$$

For the nonlinear description, define the “amplitudes” to be precisely

$$x = \langle \mathbf{z}_x^0, \mathbf{u} \rangle, \quad y = \langle \mathbf{z}_y^0, \mathbf{u} \rangle, \quad \text{where} \quad \mathbf{z}_x^0 = \begin{bmatrix} 1/2 \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{z}_y^0 = \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \end{bmatrix}, \quad (43)$$

in terms of original variables  $\mathbf{u}$ . Using the first part of the computer algebra program listed in §4.2, a quadratic approximation to the nonlinear shape of the centre manifold is

$$\mathbf{u} = \begin{bmatrix} 2x \\ -2x + 2y \\ -3x + y + \frac{42}{5}y^2 + \frac{22}{5}xy + \frac{88}{5}x^2 + \epsilon y + \epsilon x \end{bmatrix} + \mathcal{O}(\epsilon^3 + x^3 + y^3). \quad (44)$$

The lowest order structurally stable model on the centre manifold is the following cubic model

$$\begin{aligned} \dot{x} &= -y - 2xy + 6x^2 + \epsilon x \\ &\quad - \frac{84}{5}xy^2 - \frac{44}{5}x^2y - \frac{176}{5}x^3 - 2\epsilon xy - 2\epsilon x^2 + \mathcal{O}(\epsilon^2 + x^4 + y^4), \\ \dot{y} &= x + \epsilon x + \mathcal{O}(\epsilon^2 + x^4 + y^4). \end{aligned} \quad (45)$$

As is generally the case in Hopf bifurcations, with these correct cubic nonlinearities this model is usefully predictive. Numerical simulations show the birth of a limit cycle as  $\epsilon$  crosses through zero. Here we have systematically reduced the dynamics by a small step down from 3-D to a 2-D model. In serious applications to very high dimensional dynamics, we would have reduced enormously the dimensionality of the dynamics.

## 4.2 Projection onto oscillating dynamics

In this subsection I first generalise the iterative algorithm presented in §3.1 to the case of oscillatory dynamics on the centre manifold. To illustrate the algorithm and the typical results I then apply it to the simple dynamical system (39).

Restart the generic nonlinear analysis from (28). The right-hand side is just the residual of the projected dual equation (14); it stays the same. The operator on the left-hand side has to be simplified, but not as drastically as in §3.1.

- The third term  $\langle \mathcal{D}\tilde{\mathbf{z}}'_j, \mathbf{e}_k \rangle \tilde{\mathbf{z}}_k$  only changes that part of the left-hand side in the space spanned by  $\{\tilde{\mathbf{z}}_k\}$ . But we do not solve the dual (12) in this space, hence the projection seen in (14). Thus this term is safely ignored.
- The inner product in the second term of (28) simplifies under approximation as follows.

$$\begin{aligned} \langle \mathcal{D}\tilde{\mathbf{z}}_j, \mathbf{e}_k \rangle &\approx \langle \mathcal{D}\tilde{\mathbf{z}}_j, \mathbf{e}_k^0 \rangle \quad \text{as } \mathbf{e}_k \approx \mathbf{e}_k^0 \\ &\approx \langle \mathcal{L}^\dagger \mathbf{z}_j^0, \mathbf{e}_k^0 \rangle \quad \text{neglecting small terms} \\ &= \langle \mathcal{G}_{j\ell} \mathbf{z}_\ell^0, \mathbf{e}_k^0 \rangle \quad \text{using (42)} \\ &= \mathcal{G}_{jk} \quad \text{as } \langle \mathbf{z}_\ell^0, \mathbf{e}_k^0 \rangle = \delta_{\ell k}. \end{aligned}$$

- The first term, the dual operator, approximates to the homological operator

$$\mathcal{D}\mathbf{z}'_j = (\mathcal{G}_{k\ell} s_\ell + g_k) \frac{\partial \mathbf{z}'_j}{\partial s_k} + \mathcal{J}^\dagger \mathbf{z}'_j \approx \mathcal{G}_{k\ell} s_\ell \frac{\partial \mathbf{z}'_j}{\partial s_k} + \mathcal{L}^\dagger \mathbf{z}'_j.$$

Thus in general we solve

$$-\mathcal{G}_{k\ell} s_\ell \frac{\partial \mathbf{z}'_j}{\partial s_k} - \mathcal{L}^\dagger \mathbf{z}'_j + \mathcal{G}_{jk} \mathbf{z}'_k = \mathcal{D}\tilde{\mathbf{z}}_j - \langle \mathcal{D}\tilde{\mathbf{z}}_j, \mathbf{e}_k \rangle \tilde{\mathbf{z}}_k, \quad (46)$$

for the corrections to the projection vectors.

The complicating feature of (46) is that it is a coupled set of equations for the correction vectors  $\mathbf{z}'_j$ —coupled through  $\mathcal{G}_{jk} \mathbf{z}'_k$ —and that it is to be solved in the space of multinomials in the amplitudes  $\mathbf{s}$ —because of the structure of the homological operator. As noted earlier, in the iteration we may ignore components in  $\mathbf{z}_j^0$ , but we must enforce orthogonality via the iterative correction (27). Other than these complications the outline of the iterative algorithm is the same as in the previous section.

For the specific dynamical system (39) a REDUCE computer algebra program follows. Observe that the first part of the program computes the description of the centre manifold model. It is the second part that determines the projection.

```

1 COMMENT Use iteration to form the centre manifold model of an
2 elementary Hopf bifurcation problem. Then compute the projection
3 of initial conditions onto the centre manifold by iteration.
4 ;
5 % formating for printed output
6 on div; off allfac; on revpri; factor del;
7 procedure dfv(v,t); % patch differentiation of vectors
8   mat((df(v(1,1),t)),(df(v(2,1),t)),(df(v(3,1),t)));
9 procedure dfm(z,t); % patch differentiation of matrices
10  mat((df(z(1,1),t),df(z(1,2),t))
11    ,(df(z(2,1),t),df(z(2,2),t))
12    ,(df(z(3,1),t),df(z(3,2),t)));
13 %%%%%%%%
14 % PART 1: find the centre manifold
15 % matrix of linear terms and centre eigen-vectors
16 ll:=mat((-1+del*eps,-1,0),(2,1,0),(1,2,-1));
17 ex0:=mat((2),(-2),(-3));
18 ey0:=mat((0),(2),(1));
19 %
20 % only retain terms up to order o in x, y & eps
21 % use del to count the number of x, y & eps factors in a term
22 o:=3; let del^4=>0;
23 %
24 % linear solution
25 u:=del*(x*ex0+y*ey0);
26 g:=mat((-y),(x));
27 depend x,t; let df(x,t) => g(1,1);
28 depend y,t; let df(y,t) => g(2,1);
29 %
30 % iteration
31 % set arbitrary multinomial & its coefficients for later use
32 operator c;
33 hd:=for m:=0:o sum for n:=0:o-m sum c(m,n)*x^m*y^n$
34 clist:={}
35 for m:=0:o do for n:=0:o-m do clist:=c(m,n).clist$
36 repeat begin
37   % compute residual of ODEs
38   ru:=dfv(u,t); ru:=-ru+ll*u+mat((-2),(2),(0))*u(1,1)*u(3,1)
39   +mat((0),(0),(1))*u(2,1)^2;
40   % solve first two components for evolution g
41   gd:=mat((ru(1,1)),(ru(1,1)+ru(2,1)))/2/del;
42   write g:=g+gd;
43   % form and solve homological equation
44   eqn:=hd-y*df(hd,x)+x*df(hd,y)-(ru(3,1)-(-3*gd(1,1)+gd(2,1))*del);

```

```

45      elist:={} ; for m:=0:o do for n:=0:o-m do
46          elist:=coeffn(coeffn(eqn,x,m),y,n).elist;
47          write u:=u+mat((0),(0),(sub(solve(elist,clist),hd)));
48 end until (ru=mat((0),(0),(0)));
49 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
50 % PART 2: compute the vectors zx & zy to give projection onto CM
51 % adjoint jacobian and tangent vectors
52 ja:=tp(l1+mat((-2*u(3,1),0,-2*u(1,1))
53           ,(2*u(3,1),0, 2*u(1,1)),(0,2*u(2,1),0)))$ 
54 z0:=mat((1/2,1/2),(0,1/2),(0,0));
55 es:=mat((df(u(1,1),x),df(u(1,1),y))
56           ,(df(u(2,1),x),df(u(2,1),y))
57           ,(df(u(3,1),x),df(u(3,1),y)))/del$
58 % truncate approx & form arbitrary multinomials & coefficients
59 o:=2; let del^3>0;
60 zxd:=for m:=0:o sum for n:=0:o-m sum c(m,n,1)*x^m*y^n$
61 zyd:=for m:=0:o sum for n:=0:o-m sum c(m,n,2)*x^m*y^n$
62 clist:={}$
63 for m:=0:o do for n:=0:o-m do clist:=c(m,n,1).(c(m,n,2).clist)$
64 % initial linear approx, then iterate
65 z:=z0$
66 repeat begin
67     % compute residuals of the projected dual and orthogonality
68     dz:=dfm(z,t); dz:=dz+ja*z;
69     rdz:=dz-z*(tp(es)*dz);
70     rze:=mat((1,0),(0,1))-tp(z)*es;
71     % form and solve homological equation from 3rd component
72     eqx:= zxd+y*df(zxd,x)-x*df(zxd,y)-zyd -rdz(3,1);
73     eqy:= zyd+y*df(zyd,x)-x*df(zyd,y)+zxd -rdz(3,2);
74     elist:={}$ for m:=0:o do for n:=0:o-m do
75         elist:=coeffn(coeffn(eqx,x,m),y,n).
76             (coeffn(coeffn(eqy,x,m),y,n).elist);
77     csoln:=solve(elist,clist);
78     % update approx
79     write z:=z+z0*tp(rze)
80           +mat((1),(-1/2),(1))*mat((sub(csoln,zxd),sub(csoln,zyd)));
81 end until (rdz=mat((0,0),(0,0),(0,0)))and(rze=mat((0,0),(0,0)));
82 end;

```

Observe how the second part of this program implements the algorithm, in lines 50–81.

1.  $\ell_{14-48}$  compute the centre manifold (44) and the model evolution (45) using the iterative algorithm of [27]. Note that REDUCE does not implement matrices well and so  $\ell_{7-12}$  define two procedures to help.
2.  $\ell_{51-65}$  is initialisation.

- $\ell_{52-53}$  computes the adjoint operator  $\mathcal{J}^\dagger$  on  $\mathcal{M}_c$ .
- $\ell_{54}$  sets the linear projection vectors  $z_j^0$  into a  $3 \times 2$  matrix.

- $\ell55\text{--}57$  computes the tangent vectors  $\mathbf{e}_j$  of  $\mathcal{M}_c$ .
- $\ell59$  says to truncate the computations to have errors  $\mathcal{O}(\delta^3)$  as these should be accurate enough and will speed computation.
- $\ell60\text{--}63$  define general multinomial expressions and a list of their coefficients for later use in solving the homological equation via the method of undetermined coefficients.
- $\ell65$  sets  $\mathbf{z}_j$  to its initial approximation.

3.  $\ell66\text{--}81$  perform the iterations until the residuals of the desired equations are zero to the order of error specified.

- $\ell68\text{--}70$  computes the residuals of the projected dual equation (14) and the orthonormality condition (13), assigned to `rdz` and `rze` respectively.
- $\ell72\text{--}77$  solves for the undetermined coefficients of the corrections using the third component of equation (46). The first term on the right-hand side of  $\ell70$ , for example, comes from  $-\mathcal{L}^\dagger \mathbf{z}'_j$ ; the second and third terms represent  $-\mathcal{G}_{k\ell} s_\ell \frac{\partial \mathbf{z}'_j}{\partial s_k}$ ; while the fourth term comes from  $\mathcal{G}_{jk} \mathbf{z}'_k$ ; and the last term is from the residual.
- $\ell79\text{--}80$  updates the approximation to better satisfy the orthonormality and the projected dual.

The output of this computer program indicates that projections from initial conditions off  $\mathcal{M}_c$  onto  $\mathcal{M}_c$  are to be orthogonal to

$$\mathbf{z}_x \approx \begin{bmatrix} \frac{1}{2} & +\frac{2}{5}y - \frac{6}{5}x & -\frac{26}{25}y^2 - 4xy + \frac{714}{25}x^2 - \frac{28}{25}\epsilon y + \frac{34}{25}\epsilon x \\ 0 & -\frac{1}{5}y + \frac{3}{5}x & -\frac{124}{25}y^2 + \frac{68}{5}xy + \frac{6}{25}x^2 + \frac{4}{25}\epsilon y + \frac{13}{25}\epsilon x \\ 0 & +\frac{2}{5}y - \frac{6}{5}x & +\frac{16}{5}y^2 - \frac{44}{5}xy + \frac{24}{5}x^2 - \frac{18}{25}\epsilon y + \frac{4}{25}\epsilon x \end{bmatrix}, \quad (47)$$

$$\mathbf{z}_y \approx \begin{bmatrix} \frac{1}{2} & -\frac{4}{5}y + \frac{2}{5}x & +\frac{52}{25}y^2 + \frac{74}{5}xy - \frac{238}{25}x^2 + \frac{16}{25}\epsilon y + \frac{2}{25}\epsilon x \\ \frac{1}{2} & +\frac{2}{5}y - \frac{1}{5}x & +\frac{248}{25}y^2 - \frac{16}{5}xy - \frac{2}{25}x^2 + \frac{12}{25}\epsilon y - \frac{11}{25}\epsilon x \\ 0 & -\frac{4}{5}y + \frac{2}{5}x & -\frac{32}{5}y^2 + \frac{16}{5}xy - \frac{8}{5}x^2 - \frac{4}{25}\epsilon y + \frac{12}{25}\epsilon x \end{bmatrix}. \quad (48)$$

For example, consider the dynamics from the initial condition  $\mathbf{u}_0 = (0.022, 0, 0.073)$  and the corresponding evolution on  $\mathcal{M}_c$ . According to either the leading order projection or the definition of the amplitudes  $x$  and  $y$ , equation (43),  $\mathbf{u}_0$  corresponds to the point on  $\mathcal{M}_c$  with parameters  $x = y = 0.011$ , namely  $\mathbf{u}_0^0 = (0.022, 0, -0.019)$ . However, at this point on  $\mathcal{M}_c$  the projection of initial conditions should be slightly different; according to the linear

modifications in (47–48) it should be orthogonal to the columns of

$$\mathbf{z} = \begin{bmatrix} 0.492 & 0.496 \\ 0.004 & 0.502 \\ -0.008 & 0.004 \end{bmatrix}.$$

Thus, according to (15), a more appropriate initial condition on  $\mathcal{M}_c$  is  $\mathbf{u}_0^1 = (0.021, 0.001, -0.017)$ . Similarly, the second order corrections in (47–48) refine the initial conditions further. The differences here are rather small, but the improvement is seen in Figures 1–2. Figure 1 shows the qualitative picture of the trajectory starting at  $\mathbf{u}_0$  exponentially quickly approaching  $\mathcal{M}_c$ , but that the model is only quantitatively predictive if  $\mathbf{u}_0$  is projected correctly. Figure 2 quantifies a comparison between the various orders of approximation to the projection and demonstrates that the refined projection vectors  $\mathbf{z}_j$  do perform better.

Also recall from §2.2 that even such small corrections to the projection as we see here may have a considerably larger influence when projecting an applied forcing onto the centre manifold model.

## 5 Concluding remarks

Work in progress will show how to apply the techniques presented here to problems of more physical interest. In particular I am examining the issue of projecting initial conditions onto the lubrication model [28] of the flow of a thin film of fluid over a solid substrate. Although there are no inertia effects in the lubrication model of the dynamics, there may well be such effects in the provision of initial conditions as the fluid dynamics relaxes to lubrication flow. Additionally, the effects of substrate roughness on the flow may be determined by projecting the appropriately perturbed substrate boundary conditions.

Finding and coding the adjoint  $\mathcal{J}^\dagger$  can be a major headache, especially for problems such as free-surface fluid dynamics. I have sought approaches based directly upon the Jacobian  $\mathcal{J}$  rather than its adjoint, because then the residual driving the iteration could be determined directly and very simply from the governing equations. However, so far, the only method I have found also involves determining the equivalent of  $\mathbf{w}$ , introduced in (17), which is considerably more involved.

Throughout this paper we have addressed the projection of initial conditions and forcing, *linearly* correct in distance from the centre manifold or in forcing amplitude. If one needs to determine effects *nonlinear* in distance,

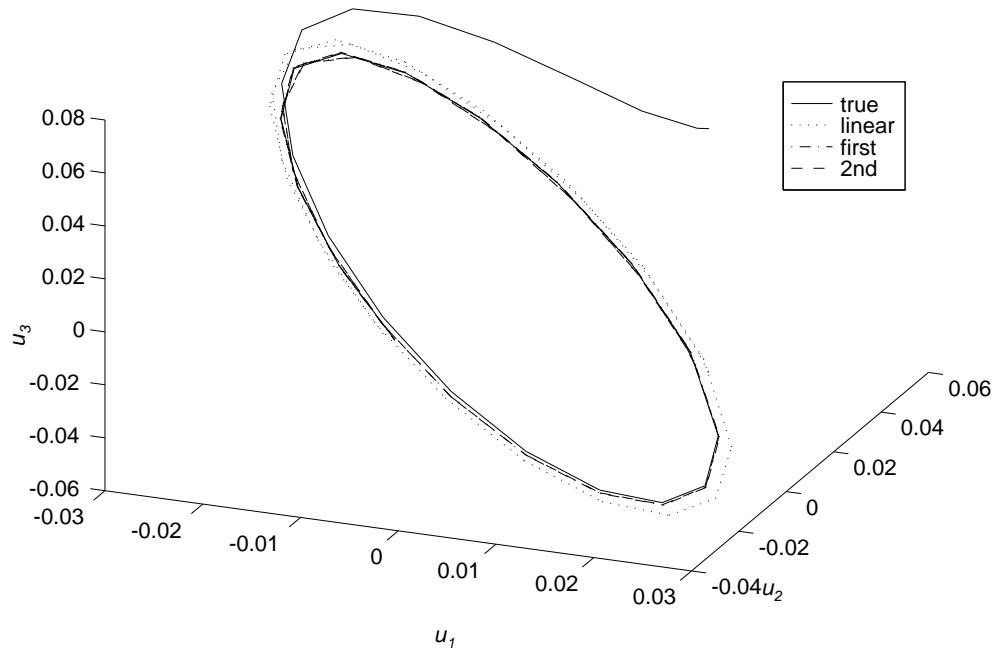


Figure 1: trajectories of (39) from the “true” initial condition of  $\mathbf{u}_0$  (solid), and from the various projections onto  $\mathcal{M}_c$ : linear from  $\mathbf{z}_j^0$  (dotted); first order (dot-dashed); second order (dashed). Observe the approximately exponential approach between the “true” and the model trajectories, but that the linearly projected trajectory is slightly awry.

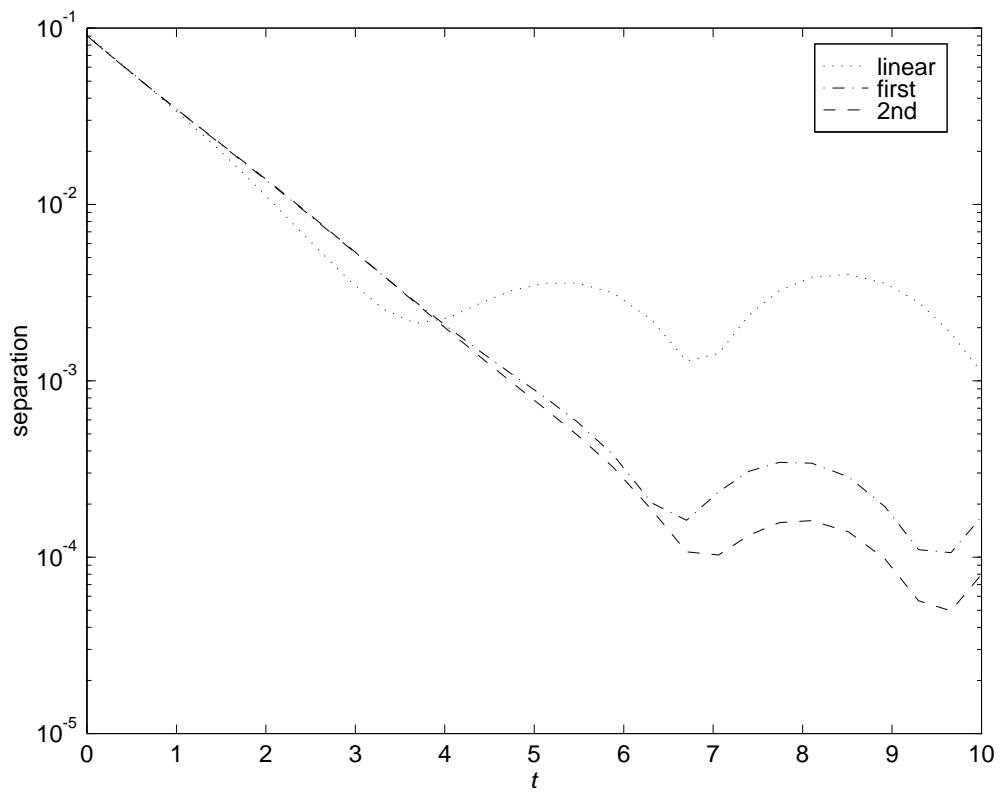


Figure 2: log of the separation between the trajectories shown in Figure 1 and the “true” solution: linear from  $z_j^0$  (dotted); first order (dot-dashed); second order (dashed). Observe the initial exponential approach, but that the first order and second order approximations to the initial conditions of the model are an order of magnitude better.

then a more sophisticated analysis is needed. At this stage the only approach I can imagine also involves the considerable labour of finding  $\mathbf{w}$ .

Lastly, Muncaster and Cohen [21, 6] suggested the construction of the low-dimensional manifold of slow, rigid-body dynamics by neglecting rapidly oscillating modes. An extremely simple example of the motion of a one-dimensional elastic body is discussed in [25, §2]. In contrast to the rapid collapse to the centre manifold, the slow dynamics on the slow manifold form a low-dimensional model because they act as a “centre” for the fast oscillations of neighbouring trajectories. This principle of neglecting fast oscillations is precisely equivalent to the guiding centre principle of Van Kampen [31]. The algebra needed to develop slow manifold models is identical to that presented here and in [27]. The algebra to model initial conditions will also be the same. However, slow manifolds are much more delicate. Cox & I [9, 10] used normal forms to show that the dynamics on and off the slow manifold generally differ by an amount of  $\mathcal{O}(\varepsilon^2)$ , where  $\varepsilon$  measures the amplitude of the fast oscillations, it measures the distance off  $\mathcal{M}_0$ . That is, generically there is some unavoidable slip between a slow model and the fully detailed oscillating dynamics.

## References

- [1] D. Armbruster, J. Guckenheimer, and P. Holmes. Kuramoto sivashinsky dynamics on the centre-unstable manifold. *Siam J Appl Math*, 49:676–691, 1989.
- [2] J. Carr. *Applications Of Centre Manifold Theory*, volume 35 of *Applied Math Sci*. Springer-Verlag, 1981.
- [3] Xu Chao and A.J. Roberts. On the low-dimensional modelling of Stratonovich stochastic differential equations. *Physica A*, 225:62–80, 1996.
- [4] M. Cheng and H.C. Chang. Subharmonic instabilities of finite amplitude monochromatic waves. *Phys Fluids A*, 4:505–523, 1992.
- [5] S.N. Chow and K.N. Lu.  $C^k$  centre unstable manifolds. *Proc Roy Soc Edin A*, 108:303–320, 1988.
- [6] H. Cohen and R.G. Muncaster. The theory of psuedo-rigid bodies. *Springer Tracts In Natural Philosophy*, 33, 1988.
- [7] P.H. Coullet and E.A. Spiegel. Amplitude equations for systems with competing instabilities. *SIAM J. Appl. Math.*, 43:776–821, 1983.

- [8] S.M. Cox and A.J. Roberts. Centre manifolds of forced dynamical systems. *J. Austral. Math. Soc. B*, 32:401–436, 1991.
- [9] S.M. Cox and A.J. Roberts. Initialisation and the quasi-geostrophic slow manifold. Submitted, 1994.
- [10] S.M. Cox and A.J. Roberts. Initial conditions for models of dynamical systems. *Physica D*, 85:126–141, 1995.
- [11] C. Foias, M.S. Jolly, I.G. Kevrekidis, G.R. Sell, and E.S. Titi. On the computation of inertial manifolds. *Phys. Lett. A*, 131:433–436, 1988.
- [12] C. Foias, M.S. Jolly, I.G. Kevrekidis, and E.S. Titi. On some dissipative fully discrete nonlinear galerkin schemes for the kuramoto–sivashinsky equation. *Phys Lett A*, 186(1):87, 1994.
- [13] U. Geigenmüller, U.M. Titulaer, and B.U. Felderhof. Systematic elimination of fast variables in linear systems. *Physica A*, 119:41–52, 1983.
- [14] H. Grad. Asymptotic theory of the boltzmann equation. *Phys. Fluids*, 6:147–181, 1963.
- [15] J. Guckenheimer. Isochrons and phaseless sets. *J. Math. Biol.*, 1:259–273, 1975.
- [16] F. Haake and M. Lewenstein. Adiabatic drag and intial slip in random processes. *Phys. Rev. A*, 28:3060–3612, 1983.
- [17] E.N. Lorenz. On the existence of a slow manifold. *J Atmos Sci*, 43:1547–1557, 1986.
- [18] M. Luskin and G.R. Sell. Approximation theories for inertial manifolds. *Math Model & Num Anal*, 23:445–461, 1989.
- [19] M. Marion and R. Temam. Nonlinear galerkin methods. *SIAM J Numer Anal*, 26(5):1139–1157, 1989.
- [20] G.N. Mercer and A.J. Roberts. A complete model of shear dispersion in pipes. *Jap. J. Indust. Appl. Math.*, 11:499–521, 1994.
- [21] R.G. Muncaster. Invariant manifolds in mechanics ii: Zero-dimensional elastic bodies with directors. *Arch. Rat. Mech. Anal.*, 84:375–392, 1983.
- [22] A.J. Roberts. Appropriate initial conditions for asymptotic descriptions of the long term evolution of dynamical systems. *J. Austral. Math. Soc. B*, 31:48–75, 1989.

- [23] A.J. Roberts. The utility of an invariant manifold description of the evolution of a dynamical system. *SIAM J. Math. Anal.*, 20:1447–1458, 1989.
- [24] A.J. Roberts. Low-dimensionality—approximations in mechanics. In J. Noye and W. Hogarth, editors, *Computational Techniques and Applications: CTAC-89*, pages 715–722. Hemisphere, 1990.
- [25] A.J. Roberts. The invariant manifold of beam deformations. part 1:the simple circular rod. *J. Elas.*, 30:1–54, 1993.
- [26] A.J. Roberts. Low-dimensional modelling of dynamical systems. preprint, USQ, February 1997.
- [27] A.J. Roberts. Low-dimensional modelling of dynamics via computer algebra. *Comput Phys Comm*, 100:215–230, 1997.
- [28] R. Valery Roy, A.J. Roberts, and M.E. Simpson. A lubrication model of coating flows over a curved substrate in space. preprint, USQ, August 1996.
- [29] R. Temam. Do inertial manifold apply to chaos? *Physica D*, 37:146–152, 1989.
- [30] R. Temam. Inertial manifolds. *Mathematical Intelligencer*, 12:68–74, 1990.
- [31] N.G. van Kampen. Elimination of fast variables. *Physics Reports*, 124:69–160, 1985.
- [32] S.D. Watt and A.J. Roberts. The accurate dynamic modelling of contaminant dispersion in channels. *SIAM J Appl Math*, 55(4):1016–1038, 1995.
- [33] S. Wiggins. *Introduction to applied nonlinear dynamical sytems and chaos*. Springer-Verlag, 1990.
- [34] A. Winfree. Patterns of phase compromise in biological cycles. *J. Math. Biol.*, 1:73–95, 1974.